AERONAUTICAL SYSTEMS CENTER
MAJOR SHARED RESOURCE CENTER

CHECKPOINT/RESTART
USER'S GUIDE

September 15, 2004

Release Notes

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1. Introduction

This document defines checkpoint/restart (CP/R) at both the batch-level and application-level. For application-level CP/R, this document describes how this capability can benefit the user when using applications within the Aeronautical Systems Center (ASC) Major Shared Resource Center (MSRC) high performance computing (HPC) environment.

1.1 Assumed Background of the Reader

It is assumed that the reader of this guide has read the *ASC MSRC User's Guide*, which contains site specific information about the ASC MSRC. The *ASC MSRC User's Guide* and all other user documentation can be downloaded and viewed from our website at http://www.asc.hpc.mil/customer/userdocs/ or by contacting the ASC MSRC Service Center at 1-888-MSRC-ASC (1-888-677-2272), (937)255-0194, or DSN 785-0194.

1.2 Definition of CP/R

CP/R is the ability to restart an application from a save point that is defined either by the system or the application.

1.2.1 Batch-Level CP/R

Batch-level CP/R is a system's ability to save the state of running jobs and, at some later time (i.e. after a downtime), restart the saved jobs from the point already reached, without starting from the beginning. This requires cooperation between both the operating system and the batch-scheduler system. Due to node complexities, many systems do not implement batch-level CP/R. Also, use of this method at the ASC MSRC is not encouraged for the reasons listed in section 1.3 of this document.

Please note that batch-level CP/R is performed independently of application-level CP/R. Both methods can be used in conjunction with each other, provided both the operating system and batch job scheduler support CP/R.

1.2.2 Application-Level CP/R

Application-level CP/R is the ability of a software package to generate its own restart file. This file is commonly used to manually restart a job in the event a system crashes or a job does not finish in the requested walltime. Restart files are commonly used to chain long-running jobs together by starting a new run from the output (restart file) of a previous run.

While application-level CP/R will not automatically restart in the event of a system crash, users have more flexibility and choices in what happens with their jobs and job results. The use of application-level CP/R is highly encouraged in applications that support it.

1.3 Batch-level CP/R Availability

Below is a per system breakdown of CP/R viability at the ASC MSRC:

- **COMPAQ SC-40/45 - Unavailable:** Incompatibilities between the batch system and the operating system make batch-level CP/R impossible on this system.

- **SGI Origin 3900 - Available w/constraints:** Load Sharing Facility (LSF) on the SGI Origin 3900 can utilize CP/R; however, this practice is highly discouraged for the following reasons:

  - It cannot be done ad hoc, jobs must be specifically set up for this prior to submission.

  - Message Passing Interface (MPI) jobs take extra pre-submission steps.

  - The process has a potential to produce large files, many of which are not owned by the user.

  - These files must be created on workspace and made immune from the file scrubber.

  - Restarting requires either superuser intervention or editing of root-owned LSF configuration files.

  - There are no guarantees of success, despite the process's seeming robustness.

  - Software requiring licenses will not restart.

  - Large memory use may cause unacceptable amount of time required to write restart files.

Please contact the ASC MSRC Service Center if you believe that batch job scheduler controlled checkpointing is required for running your jobs.

2. Application-Level CP/R Capability

Applications listed in Table 1 have been identified as possessing some level of CP/R capability. Information on how to locate CP/R documentation for the identified applications has also been provided in Table 1. Please note that access to some documentation requires the user to be logged into the ASC MSRC environment. Some vendors require us to restrict access to certain applications and their documentation. These instances have been noted in the "Comments" column of the table.

Note: Implementation of checkpointing does not guarantee success during the restart process due to the type of computations being performed, method of parallel communications, and several other runtime variations that exist within the execution of an application.

Table 1: Applications Having CP/R Capibility

Application Name	Documentation Location	Comments
Abaqus	On-line Method: 1) On any HPC system, type "abaqus doc". 2) In the "Book Titles" section, double click on "ABAQUS Keywords Manual". 3) Click on "R" to expand the R's. 4) Find "RESTART" and click to expand "RESTART". 5) Select topic of interest: "Using RESTART in an ABAQUS/Standard anlysis" or "Using RESTART in an ABAQUS/Explicit analysis". Browser Method: 1) From a web browser opened from an HPC or SciVis system, open the file "/app/abaqus/documentation/html-doc/ V6.3__HTMLdocs/index.html" 3) Click on "R" to expand the R's. 4) Find "RESTART" and click to expand "RESTART". 5) Select topic of interest: "Using RESTART in an ABAQUS/Standard anlysis" or "Using RESTART in an ABAQUS/Explicit analysis".	ASC MSRC access required to access documentation.
ACES II	http://www.qtp.ufl.edu/Aces2/aces2man_13.html	
AMSOL	http://comp.chem.umn.edu/amsol/man.txt	
Cerius2	http://www.accelrys.com/doc/	Server codes only. Documentation is password protected; please contact the ASC MSRC Service Center for more information.
Cobalt (CHSSI)	See examples in /app/cobalt/example/	ASC MSRC access required to access documentation. Application has restricted access; please contact the ASC MSRC Service Center for more information.

Table 1: Applications Having CP/R Capibility

Application Name	Documentation Location	Comments
Cobalt (Commercial)	/app/cobalts/reference/Refmanual.pdf	ASC MSRC access required to access documentation. Application has restricted access; please contact the ASC MSRC Service Center for more information.
Crystal	http://www.asc.hpc.mil/software/info/crystal/manual98.pdf	
CTH	/app/cth/doc/cth/cth.pdf or /app/cth/doc/cth/cth.ps	ASC MSRC access required to access documentation. Application has restricted access; please contact the ASC MSRC Service Center for more information.
DL_POLY	http://hidra.iqfr.csic.es/man/dlpoly/USRMAN/ node106.html	
FMD	http://www.asc.hpc.mil/software/info/fmd/fmd_ug.php	
GAMESS	http://www.asc.hpc.mil/software/info/gamess/doc/input.txt	
GASP	/app/gasp/doc/gasp4-manual.pdf (See section 4.1)	ASC MSRC access required to access documentation. Application has restricted access; please contact the ASC MSRC Service Center for more information.
Gaussian	http://www.gaussian.com/g_ur/keywords.htm	
Insight II	http://www.accelrys.com/doc/	Server codes only. Documentation is password protected; please contact the ASC MSRC Service Center for more information.
Jaguar	http://www.asc.hpc.mil/software/info/jaguar/manual/ 4.1_manual_complete.html	
LAMMPS	http://www.asc.hpc.mil/software/info/lammps/doc/ README.html	
LSDYNA 3D	1) On any HPC system, type "lsdyna3d manual". 2) Open the "ls-dyna_970_manual_k.pdf" file. 3) In the "Bookmark" section select "Restart Input Data".	ASC MSRC access required to access documentation.
LSDYNA 3D MPI	1) On any HPC system, type "lsdyna3d manual". 2) Open the "ls-dyna_970_manual_k.pdf" file. 3) In the "Bookmark" section select "Restart Input Data".	ASC MSRC access required to access documentation.
Materials Studio	http://www.accelrys.com/doc/	Server codes only. Documentation is password protected; please contact the ASC MSRC Service Center for more information.
MOLPRO	http://www.molpro.net/current//doc/manual/node578.html Search for the keyword RESTART	

Table 1: Applications Having CP/R Capibility

Application Name	Documentation Location	Comments
Mopac	http://www.schrodinger.com/Documents/mopac2000.pdf	
MSU Turbo	http://WWW.ERC.MsState.Edu/simcenter/docs/ msu_turbo/input.doc.P_V.3.html#restart_flag	
NWChem	http://www.asc.hpc.mil/software/info/nwchem/ user.001.pdf	
OVERFLOW-D2	/app/overflow/doc/overflowd/input.ps	ASC MSRC access required to access documentation. Application has restricted access; please contact the ASC MSRC Service Center for more information.
Q-Chem	http://www.asc.hpc.mil/software/info/qchem/guide2_0.pdf	
TBMD	http://cst-www.nrl.navy.mil/~mehl/tbmd/key-words.html#SECTION000518100000000000000	
VASP	http://www.asc.hpc.mil/customer/userdocs/vendor/vasp/ html/node104.html -or- http://www.asc.hpc.mil/customer/userdocs/vendor/vasp/ vasp_letter.ps (page 54)	
WIND	http://www.grc.nasa.gov/WWW/winddocs/user/keywords/ restart.html	

*NOTE: Copying URLs and pasting them into a web browser will cause spaces to be created wherever a line-wrap occurs. If you are getting Page Not Found errors, search the URL you pasted for spaces.

3. CP/R Alternatives for "Homegrown" Codes

Many users create their own programs to run at the ASC MSRC. The majority of those "homegrown" codes also utilize restart files to help with long-running jobs and system downtimes.

Restart files allow the user to restart a new job using the output or restart file of a previous job. This is the most commonly used method of restart used at the ASC MSRC.

If your application does not write restart files, you may wish to investigate adding this functionality to your code. Restart file capabilities generally works best with iterative methods, since a restart file can be potentially written after each iteration stops. In most situations, analytical codes require the analysis to run to completion, making restart capabilities difficult to incorporate, if not impossible.

When adding this feature to your application, you should:

- Store only critical information. Some things, such as operators, are derivable from inputs and need not be stored. Operands or other results of the iterative step, which have changed since the beginning of the run, are good candidates for storing in restart files.
- Determine how often to create a restart file. This will vary depending on the amount of processor time required for an iteration. Since the purpose of a restart file is to continue from a known position in the calculation, one should balance the amount of time spent on recalculating with the amount of time spent writing the restart file.
- Use unformatted (binary) reads/writes of restart files to save space and time spent on storing/restoring data.
- Have a means of distinguishing a run from initial condition and one starting after a number of steps have been computed.

Given the differences in programming style and user preference, it is impossible to give specific details and examples on what to add to your code to give it restart file capabilities. If you require assistance, please contact the ASC MSRC Service Center.

4. Customer Service

4.1 Customer Service Center

For customer assistance, call the ASC MSRC Service Center at 1-888-MSRC-ASC (1-888-677-2272), (937) 255-0194, or DSN 785-0194, or send e-mail with a description of the problem to msrchelp@asc.hpc.mil. The support analysts will help with anything related to ASC MSRC: third party software, UNIX, the different ASC MSRC computers, etc. If you have any questions about the ASC MSRC, contact the Service Center first. If your problem or question is beyond the scope of their expertise, they will refer you to the appropriate resource.

4.2 ASC MSRC Support

In-depth technical inquiries and problems are forwarded to the ASC MSRC Customer Assistance and Technology Center (CATC), which pursues such inquiries and problems through resolution as rapidly as possible. The ASC MSRC CATC will attempt to determine the nature of the problem, then identify and coordinate whatever resources are needed to resolve the problem.

The ASC MSRC also offers training classes, which provide an introduction to UNIX and the ASC MSRC. Intermediate and advanced classes on selected topics are also periodically announced on the Programming Environment and Training (PET) section of the ASC MSRC homepage. Topics for such classes may be requested through the Customer Service Center.

The ASC MSRC CATC is ready to support in an advisory capacity any engineer or scientist who is (or potentially is) an ASC MSRC user.

4.3 ASC MSRC Website

The ASC MSRC website is the best source for current ASC MSRC information. To access the ASC MSRC website simply access this URL: http://www.asc.hpc.mil.

Some of the topics found on the website include:

APPLICATIONS
Short and long descriptions of current ASC MSRC applications
http://www.asc.hpc.mil/software/

SYSTEMS
Information on ASC MSRC servers and Archival Storage
http://www.asc.hpc.mil/hardware/

CUSTOMER SERVICE
Available Customer Services
http://www.asc.hpc.mil/customer/

ONLINE DOCUMENTATION
Listings of the ASC MSRC User Guides are available for viewing. Instructions are given on obtaining postscript versions.
http://www.asc.hpc.mil/customer/userdocs/

VISUALIZATION LAB INFORMATION
Current status and other information about the Visualization Lab.

http://www.asc.hpc.mil/sciviz/

TRAINING

Current course offerings and schedule
http://www.asc.hpc.mil/education/training/

FREQUENTLY ASKED QUESTIONS

Submit questions and read about various topics (such as "Customizing Your Environment")
http://www.asc.hpc.mil

POLICIES AND PROCEDURES

The latest policies regarding usage of the ASC MSRC resources.
http://www.asc.hpc.mil/overall/policy_procedure/